MOCUP Documentation

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INTRODUCTION

For computing the growth and decay of radioactive nuclides, the ORIGEN-S code can be very useful. However, it has shortcomings that prevent it from being applied in all situations. ORIGEN only uses activation product libraries for a small list of nuclear reactor geometries. It cannot be used for the activation of an arbitrarily-shaped sample by a custom flux of neutrons. This prevents one from using ORIGEN to simulate an active interrogation experiment, for example.

Hence, a tool called MOCUP has been created. This program couples ORIGEN 2.2 and MCNP in order to simulate the growth and decay of radionuclides in arbitrary geometries. In the past, MOCUP used the now-outdated ORIGEN 2.2 decay libraries, which have been upgraded to the current versions found with ORIGEN-S.

REQUIRED FILES

In order to run MOCUP, one must have access to a computer running Linux with C-shell and MCNP. The tool interface is composed of 4 C-shell scripts, which control the execution of a set of 3 other modules. The scripts are:

- **mocup**: Executes the toolchain for a given number of irradiation / decay cycles (time steps). The number of time steps is controlled by the st variable set in the script
- **mocupRUN**: Calls MCNP and ORIGEN for each time step. MCNP is used to calculate the activation and fission rates of the irradiated material, which are then used to define a starting composition for ORIGEN. Simple decay of the products also occurs in this script.
- **origen.ex**: Manages the input and output for the ORIGEN 2.2 module. Saves the TAPE# ORIGEN input and output as time-step specific files for later use.

- **run**: Calls the origen.ex process with a list of libraries to use.

The three main modules process the input and output files for each run of MCNP and ORIGEN, and are named:

- **mcnpPro**
- **origenPro**
- **compPro**

In addition, there are two data files used by MOCUP's subroutines.

- **cross.lib**: Tabulates cross-sections for a set of reactions, for a long list of known nuclides
- **nct**: A two-column list of ZAID nuclide identifiers. Both entries on a single line represent the same nuclide, though the left-hand column is in MCNP format, while the right-hand side is in ORIGEN format

The above files generally need not be modified. However, MOCUP uses 5 other files as input, 4 of which must be modified for different simulations.

- **fmt**: A single-line file that specifies the total neutron source strength. MCNP gives results in counts per source neutron, so the number given in this file allows MOCUP to scale the MCNP results accordingly.
- **inp.1**: The initial input deck for use with MCNP from the first time step. MOCUP modifies this with new composition data for each activation / decay cycle. There are several MOCUP-specific parameters to include in this file.
- **skele.1s.a**: An ORIGEN 2.2 input deck
- **skele.1.a**: An ORIGEN 2.2 input deck

If running multiprocessing on a cluster (such as the UC Berkeley DECF machines), there is one more input file to consider.

- machines: A text file for use with the multiprocessing task scheduler, PVM. Allows easy construction of a multi-node system for use with MCNP5. Note that you must modify the line in mocupRUN that calls MCNP to account for the number of nodes used. If running on a single machine, PVM need not be used, and one can simply call **"mcnp5 n=${I}.${T}"** if using MCNP5. If using N nodes, however, this line must read **"mcnp5 n=${I}.${T} tasks=Nx1"**.

Finally, note the presence of the "moi_files" folder in the MOCUP working directory. This folder is required, and should be empty before each run. It is where output is stored.

A NOTE ON THE ORIGEN 2.2 INPUT / OUTPUT TAPES

ORIGEN uses a set of TAPE files for its input and output system. Each one is numbered, according to the specific use of the file. For example, TAPE5 is the standard name given to the ORIGEN input file. Below is a list detailing which MOCUP output file corresponds to which TAPE deck.

- TAPE3.INP ---- moi.x.x.sup
- TAPE5.INP ---- moi.x.x.inp
- TAPE9.INP ---- *.lib
- TAPE10.INP ---- *.lib
- moi.x.x.out ---- TAPE6.OUT + TAPE12.OUT
- moi.x.x.u11 ---- TAPE11.OUT + TAPE13.OUT
- moi.x.x.pch ---- TAPE7.OUT
- moi.x.x.dbg ---- TAPE15.OUT
- moi.x.x.vxs ---- TAPE16.OUT
- moi.x.x.ech ---- TAPE50.OUT

The moi.x.y.* files are named after two parameters. “x” is the number of the cell in the MCNP input deck for which the composition is tracked. “y” is the number of the time step.

GENERAL EXECUTION

mocup calls mocupRun for a time step, which then calls MCNP. MCNP creates tallies of reaction rates for the various nuclides in the problem; these are the reaction rates that are due to the custom radiation source. The reaction rates are then read by mcnpPRO. This module calculates the corresponding reaction cross-sections due to the source irradiation, and passes them to origenPRO, which then prepares and runs an ORIGEN input deck for the activation phase of the time step. After some post-

processing of the activation results, ORIGEN is run again, but for the decay phase of the time step.

Unless no other time steps are specified, the output composition from the decay case is read into a new MCNP input deck, and the mocup script starts the process again for the next activation/decay cycle.

HOW TO MODIFY INPUT

As noted earlier, there are 4 main input files. The fmt file is trivial to use, leaving us with three other files to deal with.

- **inp.1**: This is the MCNP input deck that MOCUP starts the simulation with. The format is identical to the standard MCNP input, including geometry and source definitions. There are a few MOCUP-specific conventions, though.
    - The material for which the composition should be tracked needs to be defined in a special cell. To specify this "depletion cell", one must give its density in atoms per barn-cm. Non-depletion cells should have densities given in g/cm^3.
    - The material corresponding to the depletion cell should list all nuclides initially present in the sample, plus any additional nuclides for which concentrations should be tracked. Each component nuclide should have its actual concentration specified in atoms per barn-cm. The nuclides that are not initially present, but which should be tracked, should be given very low concentrations (like 1E-24 atoms per barn-cm). For example, consider the material:

```
M1 92235 0.0058877
   92238 0.0077179
   82206 1E-24
```

      This material contains significant amounts of ^{238}U and ^{235}U, which will be tracked. In addition, the amount of ^{206}Pb created through decay will also be accounted for.

    - Every component to be tracked must also have its own material definition, for use with a reaction rate tally. The format is as follows:

“mnnn ZAID 1.”, where mnnn is the material number and ZAID is the nuclide identifier. Note that the material definition line should terminate in “1.” In the above example, one should have three materials in addition to those used in the problem geometry:

```
M2 92235 1.
M3 92238 1.
M4 82206 1.
```

- Finally, one must specify tallies for reaction rates within the depletion cell. It is these tallies which allow MOCUP to calculate reaction cross-sections for the decays of the nuclides in the cell. The tally specification requires a set of comments, and the tallies themselves should be the “F4” (volume flux) type. The tally section starts with the following:

```
c    begin_mocup_flux_tallies
c    time dependent flux
fc4  volume average flux tally
f4:n
       1
c    end_mocup_flux_tallies
c
c    begin_mocup_reaction_rate_tallies
c    time dependent reaction rates
fc14  Reaction rates
f14:n
       1
```

The tally multiplier (FM) card then follows. Each tracked nuclide should have a line specified in the FM card.

```
fm14    (1   2   (16) (17)       (102))$
        (1   3   (16) (17)       (102))$
        (1   4   (16) (17)       (102))$
c     end_mocup_reaction_rate_tallies
```

The above tally multiplier applies to materials 2, 3, and 4, which in our example correspond to the materials used for ^{235}U, ^{238}U, and ^{206}Pb, respectively. The first parameter in each line gives the cell number of the tally. The other parameters (in parentheses above) are numerical designations for certain reaction types of interest. Appendix A lists the designations for the various neutron-related reactions. A complete list for all reactions can found in Appendix G of the MCNPX 6 manual.

- **skele.1s.a**: This is a skeleton ORIGEN input deck, which contains information on the irradiation steps at which nuclide concentrations should be calculated. Note that only irradiation cases can be specified in this file; decay cases are handled elsewhere. Below is a sample input file. There are a few things of import here, marked in red.

```
-1
-1
-1
TIT    BWR bundle - 9x9 (7 control rods)
BAS    BWR bundle
LIP    1 1 0
LPU    922350 922380        -1
LPU    822060               -1
LIB    0   0 2 3    0 -205 -206   9 50 0  4   0
OPTL   8 8 8 8 7  8 8 8 8 8  8 8 8 8 8  8 8 8 8 8  3 3 8 8
OPTA   8 8 8 8 7  8 8 8 8 8  8 8 8 8 8  8 8 8 8 8  3 3 8 8
OPTF   8 8 8 8 7  8 8 8 8 8  8 8 8 8 8  8 8 8 8 8  3 3 8 8
CUT    3 1.0E-24  28 1.0E-75   -1
INP    1   2  -1  -1  1  1
IRF      0.01  1.000000E+00    1    2   1   2
IRF      0.02  1.000000E+00    2    3   1   0
IRF      0.03  1.000000E+00    3    4   1   0
IRF      0.04  1.000000E+00    4    5   1   0
IRF      0.05  1.000000E+00    5    6   1   0
IRF      0.06  1.000000E+00    6    7   1   0
IRF      0.07  1.000000E+00    7    8   1   0
```

```
IRF       0.08  1.000000E+00    8    9   1   0
IRF       0.09  1.000000E+00    9   10   1   0
IRF       0.10  1.000000E+00   10   11   1   0
OUT     11  1  0  0
PCH     11  11  11
STP     4
205  922350
2    922350
0
```

- The LPU cards specify the nuclides present in the sample. The actual composition data is not included in this file, as it is automatically added later by mcnpPRO.
- In the line labeled with the keyword “INP”, the last two parameters give the dimensions of time units used in the simulation. The units are as follows:

  1: seconds

  2: minutes

  3: hours

  4: days

  5: years

  6: infinite (nuclide is stable)

  7: kiloyears

  8: megayears

  9: gigayears

- There are 10 lines beginning with the IRF keyword. Each of these signifies a length of time during which the sample is irradiated. There can be as many of these steps per input as is desired, though they must be grouped in blocks of 10 or less. Each IRF line contains several parameters. Use the following as an example:

  IRF 0.01 1.000000E+00 1 2 1 2

```
IRF       0.02   1.000000E+00     2     3     1      0
IRF       TIME       ???        START END UNITS BLOCK
```

- The "TIME" entry gives the length of the time step. In this example, the first step ends at time 0.01 and begins at time 0. The second begins at t = 0.01 and ends at t = 0.02.
- START is the index of the time step from which an initial composition should be taken. START = 1 means the initial composition input into the file should be used.
- END is the index of the time step to output composition data to. For the above irradiation steps, step #2 takes its composition data from step #1, and provides it to step #3.
- UNITS gives the units of time used in the irradiation. See the above table that links the numerical abbreviation with the unit.
- BLOCK tells whether a decay case is resuming from a previous irradiation group, or from its own t = 0. That is, if you had 20 irradiation steps, the 11th one should resume from the previous block. This parameter can be set to either 0 (continue from last step) or 2 (begin at t = 0).

- **TAPE5.INP**: This file is located in the ./decay folder within the MOCUP working directory. Like skele.1.a, it is a skeleton ORIGEN input deck. Most of it will be identical, except that the irradiation cases of skele.1.a are replaced with decay cases. One would see the format:

```
DEC       TIME       ???        START END UNITS BLOCK
```

  - Note that, even though the decay occurs after the irradiation step, this TAPE5.INP file is technically a new ORIGEN problem. The first decay step should begin at t = 0 (setting BLOCK = 2).
  - The compositions from the irradiation are automatically written to the TAPE5.INP file as needed.

DESCRIPTION OF OUTPUT

There are two important output files given per time step. Let N be the depletion cell number and M be the irradiation / decay cycle number. Then **moi.N.M.out**, located in the “moi_files” folder, contains composition data for the irradiation step. The **after_decay_full.M** file, located in the “decay” directory, lists the full ORIGEN output after the decay cases have executed.

Appendix A: Neutron Continuous-Energy and Discrete Reaction Numbers for MCNP

Reaction Number	Microscopic Cross-Section Description
-1	Total
-3	Elastic
16	(*n*,2*n*)
17	(*n*,3*n*)
-6	Total fission cross section (Equal to the sum of reactions 19, 20, 21, and 38.)
19	(*n*,*f*)
20	(*n*,*n'f*)
21	(*n*,2*nf*)
22	(*n*,*n'*α)
28	(*n*,*n'p*)
32	(*n*,*n'd*)
33	(*n*,*n't*)
38	(*n*,3*nf*)
51	(*n*,*n'*) to 1st excited state
52	(*n*,*n'*) to 2nd excited state
...	...
90	(*n*,*n'*) to 40th excited state
91	(*n*,*n'*) to continuum
−2	Absorption (Equal to the sum of reactions 102–107.)
102	(*n*,γ)
103	(*n*,*p*)
104	(*n*,*d*)
105	(*n*,*t*)
106	(*n*,^{3}He)
107	(*n*,α)